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## Some Observations on Boundary Conditions for Numerical Conservation Laws

David Kamowitz\*

#### Abstract

In this note four choices of outflow boundary conditions are considered for numerical conservation laws. All four methods are stable for linear problems. For nonlinear problems examples are presented where either a boundary layer forms or the numerical scheme, together with the boundary condition is unstable due to the formation of a reflected shock. A simple heuristic argument is presented for determining the suitability of the boundary conditions.

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#### 1 Introduction

Consider the one dimensional scalar conservation law

$$u_t + f(u)_x = 0, \qquad 0 \le x \le 1. \tag{1}$$

If

$$a(u)=\frac{\partial f}{\partial u}\geq 0,$$

then boundary data must be specified at x = 0. Since the characteristics have nonnegative slope, one cannot set a-priori boundary conditions at x = 1 [Lax73].

To compute the solution to (1) by finite differences, the interval [0,1] is discretized into M pieces each of width

$$h=\frac{1}{M}$$

and a time interval  $\Delta t > 0$  is specified. Setting

$$\lambda = \frac{\Delta t}{\Delta x},$$

a numerical scheme for solving (1) is, for each m = 1, 2, ... M - 1,

$$u_m^{n+1} = u_m^n - \lambda (\phi_{m+1/2} - \phi_{m-1/2}). \tag{2}$$

Here,

$$u_m^n = u(m\Delta x, n\Delta t),$$

the functions

$$\phi_{m+1/2} = \phi(u_{m-k+1}, u_{m-k+2}, \dots u_{m+k})$$

$$\phi_{m-1/2} = \phi(u_{m-k}, u_{m-k+1}, \dots u_{m+k-1})$$

are the numerical fluxes and

$$u(0, n\Delta t) = g(t)$$

is specified. For consistency  $\phi$  is required to satisfy

$$\phi(u,u,\ldots u)=f(u).$$

Since only the role of the boundary conditions is of interest, three point schemes will be considered. In this case,  $\phi_{m+1/2} = \phi(u_{m+1}, u_m)$  and  $\phi_{m-1/2} = \phi(u_m, u_{m-1})$ . The Courant-Friedrichs-Lewy condition requires

$$\max_{u}|a(u)\lambda|\leq 1.$$

As mentioned above, some form of artificial boundary condition is necessary at x = 1. Four choices of boundary conditions are discussed:

1. Constant Extrapolation:

$$u_{M}^{n+1} = u_{M-1}^{n+1}, (3)$$

2. Linear Extrapolation:

$$u_{M}^{n+1} = 2u_{M-1}^{n+1} - u_{M-2}^{n+1}, (4)$$

3. Quadratic Extrapolation:

$$u_{M}^{n+1} = 3u_{M-1}^{n+1} - 3u_{M-2}^{n+1} + u_{M-3}^{n+1}, (5)$$

4. Characteristic Extrapolation:

$$u_M^{n+1} = u_M^n - \lambda (f(u_M^n) - f(u_{M-1}^n)). \tag{6}$$

Note that extrapolations (3), (4) and (5) are equivalent to requiring the first, second and third derivative, respectively, to be zero at the boundary.

All four boundary conditions are stable for linear problems, see for example [GKS72]. Boundary condition (4) is of particular interest here. If  $\phi$  is a monotone function of its arguments, then [HHL76] showed that limit solutions of (2) are physical solutions of (1). They also showed that such schemes are at most first order accurate. Thus, the error using linear extrapolation is the same order as the error in the numerical method. In [AM81] this choice was shown to be stable for two dimensional explicit schemes, again for linear problems. Also, in [Pul81] this boundary condition was applied to the Euler equations.

The purpose of this note is to point out that for a number of simple and well known explicit methods boundary conditions (4) and (5) are unsatisfactory for nonlinear problems. Examples are presented where, depending upon the flux function f(u), either an artificial shock forms at the boundary or a reflected shock forms.

#### 2 Numerical Observations

In the experiments the following initial data is used:

$$u(x,0) = u_0(x) = \begin{bmatrix} 1 & x \leq p, & 0 p. \end{bmatrix}$$
 (7)

The functions f(u) are chosen so that the jump in u travels in the direction of increasing x with speed

$$s=rac{1}{2}.$$

Since  $u_0 \ge 0$  the discrete solution at time t is simply

$$u_m^n = u_0(m\Delta x - \frac{n}{2}\Delta t).$$

In particular, after N time steps, where N depends on p, the numerical solution is

$$u_{\mathrm{true}}(x,N) \equiv 1, \qquad 0 \leq x \leq 1.$$

The three choices of f are:

$$f(u) = \frac{1}{2}u, \tag{8}$$

$$f(u) = \frac{1}{2}u^2, \tag{9}$$

$$f(u) = u(u-\frac{1}{2}). \tag{10}$$

Equation (9) is known as Burgers' equation.

Experiments were run with a number of different numerical schemes. In all of the tests, h = 1/32 and the initial jump in u was at x = 3/4. For the numerical experiments, starting with the initial data in (7), 50 iterations were run and the error,

$$\epsilon^n = \left\{\sum_{m=1}^M \left(u_m^n - u_{\text{true}}(m\Delta x)\right)^2\right\}^{1/2}$$

was computed. The value of  $\lambda$  was chosen to be the smaller of the CFL condition and the stability bound. Note that  $\epsilon^{50}$  is expected to be zero — the boundary conditions should not preclude the profile from passing through.

The numerical schemes tested are:

Lax-Friedrichs: Set

$$u_m^{n+1} = \frac{1}{2}(u_{m-1}^n + u_{m+1}^n) - \frac{\lambda}{2}(f_{m+1} - f_{m-1}). \tag{11}$$

The Lax-Friedrichs scheme can be written in conservation form by setting

$$\phi(u_{m+1},u_m) = -\frac{1}{2\lambda}u_{m+1}^n + \frac{1}{2\lambda}u_m^n + \frac{1}{2}f_{m+1} + \frac{1}{2}f_m.$$

	f			
Method	$\frac{1}{2}u$	$\frac{1}{2}u^2$	$u(u-\frac{1}{2})$	
Lax-Friedrichs	0	2.0	8	
MacCormick	0	0	∞	
Lax-Wendroff	0	2.36	∞	

Table 1: Error using Linear Extrapolation

MacCormick's Method: First set

$$u_m^* = u_m^n - \lambda (f_{m+1} - f_m)$$

and then put

$$u_m^{n+1} = u_m^n - \frac{\lambda}{2} (f_{m+1} - f_m) - \frac{\lambda}{2} (f_m^* - f_{m-1}^*). \tag{12}$$

Again (12) can be written in conservation form by setting

$$\phi_{m+1/2} = \frac{1}{2}f_{m+1} + \frac{1}{2}(f_m - \lambda(f_{m+1} - f_m)).$$

Lax-Wendroff: To compute  $u_m^{n+1}$  by the Lax-Wendroff scheme, set

$$u_m^{n+1} = u_m^n - \frac{\lambda}{2} (f_{m+1} - f_{m-1}) + \frac{\lambda^2}{2} [a_{m+1/2} (f_{m+1} - f_m) - a_{m-1/2} (f_m - f_{m-1})]. \tag{13}$$

To write the scheme in conservation form set

$$\phi_{m+1/2} = \frac{1}{2}(f_{m+1} + f_m) - \frac{1}{2}\lambda a_{m+1/2}(f_{m+1} - f_m).$$

In equations (11)-(13),

$$f_m = f(u_m^n), \quad a_{m+1/2} = a(\frac{1}{2}u_m^n + \frac{1}{2}u_{m+1}^n), \quad \text{etc}$$

Tables 1 and 2 display the observed value of  $\epsilon^{50}$ . For constant and characteristic extrapolation the error was equal to zero, for each choice of f.

	f			
Method	$\frac{1}{2}u$	$\frac{1}{2}u^2$	$u(u-\frac{1}{2})$	
Lax-Friedrichs	0	0.0	8	
MacCormick	0	∞	∞	
Lax-Wendroff	0	∞	∞	

Table 2: Error using Quadratic Extrapolation

## 3 Linear and Quadratic Boundary Conditions

From Tables 1 and 2 it is clear that when linear and quadratic extrapolation is used to compute the value of  $u_M$  something fundamentally different happens when f is nonlinear. Figure 1 displays the solution for each of the 50 time steps for Burgers' equation and the Lax-Friedrichs scheme. Note that the value of  $u_{M-1}$  is fixed and that  $u_M < 0$ . The picture for the Lax-Wendroff scheme is similar. This is equivalent to overspecifying the problem data. For simplicity, only the calculations for linear extrapolation will be discussed. The quadratic case is similar.

Starting with the initial data in (7), for a finite number of time steps the boundary conditions at  $x_M$  do not affect the solution. However, when

$$u_{M-2}^n > 0$$
 and  $u_{M-1}^n = 0$  (14)

the boundary conditions do affect the character of the solution. The specific value of  $u_{M-2}^n$  will depend on the particular numerical fluxes used in (1).

When updating  $u_{M-1}^{n+1}$  using (2), the new value is

$$u_{M-1}^{n+1} = u_{M-1}^{n} - \lambda (\phi_{m+1/2} - \phi_{m-1/2})$$
$$= u_{M-1}^{n} + s_{M-1}.$$

Notice that it is the sign and magnitude of  $s_{M-1}$  which determines how the solution will behave at  $x_{M-1}$ . In successive iterations the numerical experiments indicate that the behavior of the solution is determined by the situation described in (14).

The three choices of f will be considered separately.

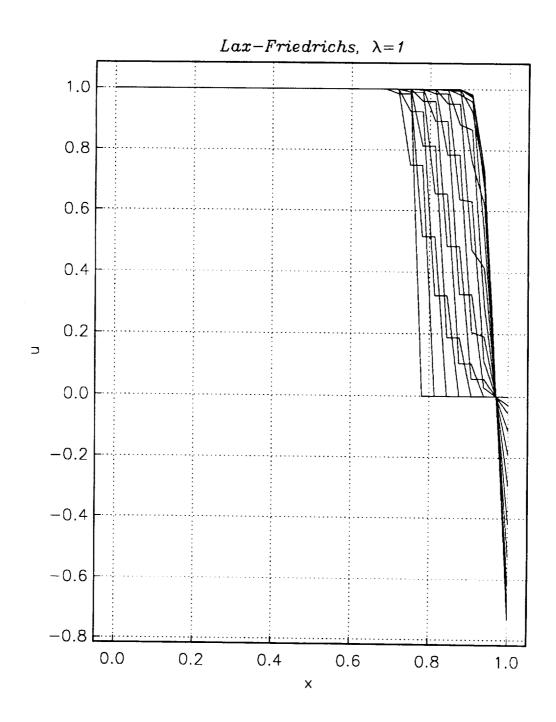


Figure 1: Burgers' Equation, Linear Extrapolation

#### 3.1 f Linear

When f is linear, in this case

$$f(u)=\frac{1}{2}u,$$

the correction for all three schemes is

$$s_{M-1}=\frac{\lambda}{2}u_{M-2}>0.$$

Here, the solution continues to travel to the right as it should.

#### 3.2 Burgers' Equation

For Burgers' equation

$$f(u)=\frac{1}{2}u^2,$$

one sees that the correction, using both the Lax-Friedrichs scheme and the Lax-Wendroff scheme, to  $u_{M-1}$  is

$$s_{M-1}=0$$

since

$$f(-u_{M-2}^n)=f(u_{M-2}^n).$$

Here an artificial boundary layer forms at  $x_{M-1}$ . Notice that the fact that  $u_{M-1} \equiv 0$  does not depend on the choice of  $\lambda$ . This same argument shows that  $u_{M-1} \equiv 0$  for all successive iterations. As  $u_{M-2} \to 1$ ,  $u_M \to -1$  and the total variation approaches 2. Note also that  $u_M < 0$  does not solve (1) since the continuous solution is positive for positive initial data.

The situation for the MacCormick scheme is different. A direct calculation shows that the difference in the numerical fluxes is

$$s_{M-1}=\frac{\lambda^2}{4}u_{M-2}^3$$

and the solution propagates to the right. For  $u_{M-2}$  small the speed of propagation is very slow. This creates a boundary layer at x = 1 for a number of time steps. Eventually, the solution does move off to the right. Figure 2 displays the solution for 50 time steps.

$$3.3 \quad f(u) = u(u - \frac{1}{2})$$

Finally, for

$$f(u)=u(u-\frac{1}{2})$$

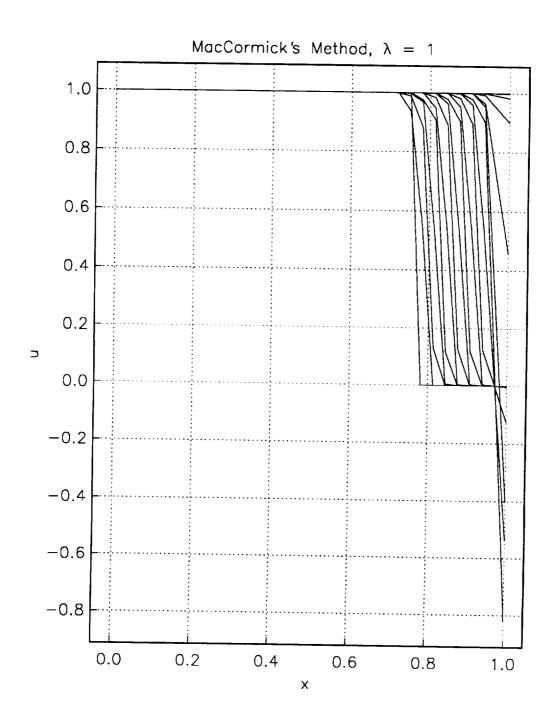


Figure 2: Burgers' Equation, Linear Extrapolation

	f		
Boundary Condition	$\frac{1}{2}u$	$\frac{1}{2}u^2$	$u(u-\frac{1}{2})$
$u_{M}^{n+1}=2u_{M-1}^{n+1}-u_{M-2}^{n+1}$	+	0	_
$u_{M}^{n+1}=u_{M-1}^{n+1}$	+	+	+
$u_M^{n+1} = u_M^n - \lambda(f(u_M^{n+1}) - f(u_{M-1}^n))$	+	+	+

Table 3: Sign of s<sub>M-1</sub>

the observations in Tables 1 and 2 indicate that the solution reflects off the boundary and that the boundary conditions are unstable.

Calculating the correction

$$s_{M-1} = -\lambda(\phi(-u_{M-2},0) - \phi(0,u_{M-2}))$$

for the three schemes yields:

$$s_{M-1}^{\text{L-F}} = -\frac{\lambda}{2}u_{M-2}^n,$$
 (15)

$$s_{M-1}^{\text{Mac}} = -\frac{\lambda}{2} [2(u_{M-2}^n)^2 \lambda^2 + (2(u_{M-2}^n)^2 - 2(u_{M-2}^n)^3) \lambda + u_{M-2}^n], \tag{16}$$

$$s_{M-1}^{\text{L-W}} = -\frac{\lambda}{2} [2(u_{M-2}^n)^2 \lambda + u_{M-2}^n].$$
 (17)

For all three methods the correction is less than zero and the computed solution diverges.

## 4 Other Boundary Conditions

The argument in Section 3 indicates that it is the speed and direction of propagation of the solution at the boundary which determines what the character of the solution will be. For the initial data in (7), Table 3 summarizes the sign of  $s_{M-1}$  for the Lax-Friedrichs scheme. The situations for MacCormick's method and the Lax-Wendroff method are similar.

Note that it is exactly those cases where  $s_{M-1} \leq 0$  that interfere with the solution propagating to the right.

### 4.1 Constant Extrapolation

When

$$u_M^n=u_{M-1}^n,$$

the correction to  $u_{M-1}^n$  reduces to evaluating

$$s_{M-1} = \phi(u_{M-1}^n, u_{M-1}^n) - \phi(u_{M-1}^n, u_{M-2}^n).$$

At each iteration

$$u_{M-2}^n \geq u_{M-1}^n$$

and since the functions  $\phi_{m\pm 1/2}$  approximate  $f(u_{M\pm 1/2})$ , the solution will continue to propagate to the right.

## 4.2 Characteristic Extrapolation

For characteristic extrapolation,

$$u_M^{n+1} = u_M^n - \lambda (f(u_m^n) - f(u_{M-1}^n)), \tag{18}$$

and the solution passes through the boundary as remarked in Section 2. Applying the above argument to compute  $s_{M-1}$  for  $u_{M-2}^n > 0$  and  $u_{M-1}^n = 0$  one sees that equation (18) implies  $u_M^n = 0$ . Evaluating the correction term to update  $u_{M-1}^n$  yields

$$s_{M-1} = -\lambda(\phi(0,0) - \phi(0,u_{M-2}^n))$$
  
 $\leq 0$ 

and  $u_{M-1}^{n+1} \geq 0$ . In this case the solution continues travelling to the right.

## 5 Concluding Remarks

In conclusion, the experimental results and the arguments in Sections 2 and 3 show that the boundary condition can have a dramatic effect on the solution. The stability analysis for linear problems does not extend to nonlinear problems and a different analysis is needed.

To address the question of what is a 'safe' outflow boundary condition, the numerical experiments show that either constant or characteristic extrapolation is suitable. Unfortunately constant extrapolation is zero order accurate with respect to the meshsize. Hence the solution at the boundary will suffer a loss of accuracy. To preserve higher order accuracy in the entire domain fictitious points will be needed. Characteristic extrapolation, while first order accurate, is more expensive to evaluate.

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